0.1 Markov Model

0.1.1 NCX Channel Inactivation Model

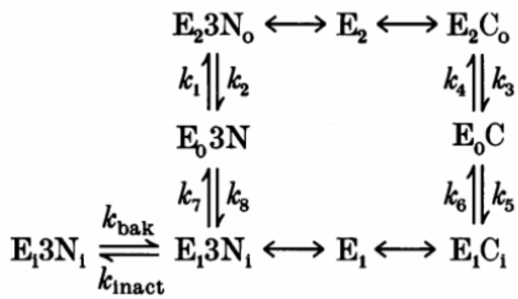

Figure 1: NCX Ion Channel Model

Notations

- E_1 : States with binding sites oriented to the cytoplasmic sides
- E_2 : States with binding sites oriented to the extra-cellular sides
- $E_1 3N_i$: States with binding sites oriented to the cytoplasmic sides containing 3 Na+ ions
- $E_0 3N$: States with binding sites occluded with 3 Na+ ions
- $E_2 3N_0$: States with binding sites oriented to the extra cellular sides with 3 Na+ ions
- $E_1 C_1$: States with binding sites oriented to the cytoplasmic sides containing 1 Ca++ ion
- $E_0 C$: States with binding sites occluded with 1 Ca++ ion
- $E_2 C_0$: States with binding sites oriented to the extra cellular sides with 1 Ca++ ion

Simultaneous Diff Equation

$$\frac{d(E_2 3N_o)}{dt} = k_1(E_0 3N) - k_2(E_2 3N_o)$$
$$\frac{d(E_0 3N)}{dt} = k_7(E_1 3N_i) + k_2(E_2 3N_o) - (k_1 + k_8)(E_0 3N)$$
$$\frac{d(E_1 3N_i)}{dt} = k_{bak}(E_i 3N_i) + k_8(E_o 3N) - (k_{inact} + k_7)(E_1 3N_i)$$
$$\frac{d(E_i 3Ni)}{dt} = k_{inact}(E_1 3N_i) - k_{bak}(E_i 3N_i)$$
$$\frac{d(E_2 C_o)}{dt} = k_4(E_o C) - k_3(E_2 C_o)$$
$$\frac{d(EoC)}{dt} = k_3(E_2 Co) + k_6(E_1 C_i) - (k_4 + k_5)(E_o C)$$
$$\frac{d(E_1 C_i)}{dt} = k_5(E_o C) - k_6(E_1 C_i)$$

Summed Version

$$\frac{d(E_1)}{dt} = k_{bak}(E_i 3N_i) + k_8(E_o 3N) + k_5(E_o C) - (k_{inact} + k_7 + k_6)(E_1)$$
$$\frac{d(E_0 3N)}{dt} = k_7(E_1) + k_2(E_2) - (k_1 + k_8)(E_o 3N)$$
$$\frac{d(EoC)}{dt} = k_3(E_2) + k_6(E_1) - (k_4 + k_5)(E_o C)$$
$$\frac{d(E_2)}{dt} = k_1(E_o 3N) + k_4(E_o C) - (k_2 + k_3)E_2$$
$$\frac{d(E_i 3N_i)}{dt} = k_{inact}(E_1) - k_{bak} E_i 3N_i$$
$$E_i 3N_i = 1 - E_1 - E_2 - E_o C - E_o 3N$$

Reduced Equation

$$\frac{d(E_1)}{dt} = k_{bak} - k_{bak}E_2 + (k_8 - k_{bak})(E_o 3N) + (k_5 - k_{bak})(E_o C)$$
$$- (k_{bak} + k_{inact} + k_7 + k_6)(E_1)$$
$$\frac{d(E_0 3N)}{dt} = k_7(E_1) + k_2(E_2) - (k_1 + k_8)(E_o 3N)$$
$$\frac{d(EoC)}{dt} = k_3(E_2) + k_6(E_1) - (k_4 + k_5)(E_o C)$$
$$\frac{d(E_2)}{dt} = k_1(E_o 3N) + k_4(E_o C) - (k_2 + k_3)E_2$$

Constants

- Gamma : $\gamma = 0.02$
- Membrane Potential : $Em = ...$
- Kem : $Kem = exp(0.5 \times (1 - \gamma) \times Em \times \frac{F}{RT}) = ...$
- Rate Constan : $k_1 = 10^4 \times Kem$
- Rate Constan : $k_2 = F_{3no} \times \frac{10^4}{Kem}$
- Rate Constan : $k_3 = F_{co} \times 5.17 \times 10^4 \times Kem$
- Rate Constan : $k_4 = 5.17 \times 10^4$
- Rate Constan : $k_5 = 5.17 \times 10^4$
- Rate Constan : $k_6 = F_{ci} \times 5.17 \times 10^4$
- Rate Constan : $k_7 = F_{3ni} \times 1.84 \times 10^4$
- Rate Constan : $k_8 = 1.84 \times 10^4 \times$
- Rate Constan : $k_{bak} = 0.12$
- Rate Constan : $k_{in} = 0.8$

0.2 Quantum Algorithms

0.2.1 Stoicheometric Correction in NCX channel

Trapped ion Quantum Computer is already in practice. There are interesting application of Quantum Physics phenomena in Quantum Biology (e.g., Photosynthesis and Mutation). In case of trapped ion, the spin of ion can be considered as a quantum qubit. In this article we want to study the interaction of three Na ions and Ca ion during the exchange process in NCX channel.